

(e)-1-(4-ethylphenyl)-2-phenyldiazene
61653-37-0 | DTXSID20295936

Model Performance

Model	Data
-------	------

Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 106

Global applicability domain: Inside

Local applicability domain index: 4.45e-01

Confidence level: 5.51e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2,2'-Dithiobisbenzothiazole</div> <div>Measured: 26.3</div> <div>Predicted: 24.5</div>	<div>Image not found</div> <div>N,N-Diethylaniline</div> <div>Measured: 102</div> <div>Predicted: 12.8</div>	<div>Image not found</div> <div>Isoamyl ether</div> <div>Measured: 170</div> <div>Predicted: 137</div>
<div>Image not found</div> <div>Disulfoton</div> <div>Measured: 219</div> <div>Predicted: 151</div>	<div>Image not found</div> <div>2-(Thiocyanomethylthio)benzothiazole</div> <div>Measured: 209</div> <div>Predicted: 13.0</div>	